Efimov physics in a finite volume

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(Dated: February 24, 2009)

Abstract

Three bosons with large scattering length show universal properties that do not depend on the details of the interaction at short distances. In the three-boson system, these properties include a geometric spectrum of shallow three-body states called "Efimov states" and log-periodic dependence of scattering observables on the scattering length. We investigate the modification of the Efimov states in a finite cubic box and calculate the dependence of their energies on the box size using effective field theory. We explicitly verify the renormalization of the effective field theory in the finite volume.

Strongly interacting quantum systems can show universal properties that are independent of the details of their interaction. These properties establish connections between systems over a wide range of scales and with different underlying interactions. One example are the hydrodynamic properties of quantum liquids. The strongly interacting quark gluon plasma created at the Relativistic Heavy Ion Collider and ultracold Fermi gases both behave as nearly perfect liquids with almost no viscosity [1]. Their viscosity to entropy density ratio is close to a lower bound that was conjectured using string theory methods [2].

Another example are universal properties in non-relativistic few-body systems [3]. Here the strong interaction regime is characterized by a large scattering length a. If a is large and positive, two particles of mass m form a shallow dimer with energy $E_2 \approx -\hbar^2/(ma^2)$, independent of the mechanism responsible for the large scattering length. Examples for such shallow dimer states are the deuteron in nuclear physics, the ⁴He dimer in atomic physics, and possibly the new charmonium state X(3872) in particle physics [3]. These systems span more than 13 orders of magnitude in energy ranging from MeV to neV. In the three-body system, the universal properties include the Efimov effect [4]. If at least two of the three pairs of particles have a large scattering length |a| compared to the range r_0 of their interaction, there is a sequence of three-body bound states whose energies are spaced geometrically between $-\hbar^2/mr_0^2$ and $-\hbar^2/ma^2$. In the limit $1/a \to 0$, there are infinitely many bound states with an accumulation point at the three-body scattering threshold. These Efimov states or trimers have a geometric spectrum [4]:

$$E_3^{(n)} = -(e^{-2\pi/s_0})^{n-n_*} \hbar^2 \kappa_*^2 / m, \tag{1}$$

where κ_* is the binding momentum of the Efimov trimer labeled by n_* . This spectrum is a signature of a discrete scaling symmetry with discrete scaling factor e^{π/s_0} . In the case of identical bosons, $s_0 \approx 1.00624$ and the discrete scaling factor is $e^{\pi/s_0} \approx 22.7$. This discrete scale invariance is also relevant if a is large but finite. It becomes manifest in the log-periodic dependence of scattering observables on the scattering length a [5]. The consequences of discrete scale invariance and Efimov physics can be calculated in an effective field theory for short-range interactions, where the Efimov effect appears as a consequence of a renormalization group limit cycle [6].

Experimental evidence for an Efimov trimer in ultracold Cs atoms was recently provided by their signature in three-body recombination rates [7]. This signature could be unravelled by varying the scattering length a over several orders of magnitude using a Feshbach resonance. More recently, evidence for Efimov trimers was also obtained in atom-dimer scattering [8] and possibly in three-body recombination in a balanced mixture of atoms in three different hyperfine states of 6 Li [9, 10].

The observation of Efimov physics in nuclear and particle physics systems is complicated by the inability to vary the scattering length. See, e.g., Ref. [11] for a recent discussion of Efimov physics in halo nuclei. Another opportunity to observe Efimov physics is given by lattice QCD simulations of three-nucleon systems [12]. A number of studies of the quark-mass dependence of the chiral nucleon-nucleon (NN) interaction found that the inverse scattering lengths in the relevant ${}^3S_1 - {}^3D_1$ and 1S_0 channels may both vanish if one extrapolates away from the physical values to slightly larger quark masses [13, 14, 15]. This implies that QCD is close to the critical trajectory for an infrared RG limit cycle in the three-nucleon sector. It was conjectured that QCD could be tuned to lie precisely on the critical trajectory by tuning the up and down quark masses separately [16]. As a consequence, the triton would display the Efimov effect. More refined studies of the signature of Efimov physics in this

case followed [17, 18]. However, a proof of this conjecture can only be given by an observation of this effect in a lattice QCD simulation [12]. The first full lattice QCD calculation of nucleon-nucleon scattering was recently reported in [19] but statistical noise presents a serious challenge and no three-nucleon calculation has been carried out to date. Since lattice simulations are carried out in a cubic box, it is important to understand the properties of Efimov states in the box. Apart from this application, the modification of Efimov physics in a finite volume is an interesting question on its own and could be tested with ultracold atoms in optical lattices.

The modifications to the Efimov spectrum can be calculated in effective field theory (EFT) since the finite volume modifies the infrared properties of the system. The properties of three-body systems in a finite volume have been studied previously. For repulsive and weakly attractive interactions without bound states, Tan has determined the volume dependence of the ground state energy of three bosons up to $\mathcal{O}((a/L)^7)$ [20]. In Refs. [21, 22], this result was extended for general systems of N bosons. First results for three and more boson systems from lattice QCD have become available recently [23, 24, 25]. For the unitary limit of infinite scattering length some studies have been carried out as well. The properties of three spin-1/2 fermions in a box were investigated in [26]. In this system, the Efimov effect does not occur due to the Pauli principle. The spectrum of three bosons in a harmonic trap was calculated by Werner and Castin [27].

In this letter, we investigate the finite volume corrections for a three-boson system with large but finite scattering length. In particular, we derive an integral equation for the trimer energies in a system of three identical bosons in a cubic box and solve this equation for a few exemplary cases. We follow the strategy proposed in [28] and extend the the EFT for the three-boson system with short-range interactions of Ref. [6] to a cubic box. We also verify explicitly that the renormalization of the EFT is not affected by the box. Our study is carried out to leading order in the large scattering length. This corresponds to the zero range limit with $r_0 = 0$. Our results will be applicable to physical states whose size is large compared to r_0 . Using units with $\hbar = m = 1$ from now on, the effective Lagrangian can be written as [3]

$$\mathcal{L} = \psi^{\dagger} \left(i \partial_t + \frac{1}{2} \nabla^2 \right) \psi + \frac{g_2}{4} d^{\dagger} d - \frac{g_2}{4} \left(d^{\dagger} \psi^2 + \text{h.c.} \right) - \frac{g_3}{36} d^{\dagger} d \psi^{\dagger} \psi + \dots,$$
 (2)

where the dots indicate higher order terms. It involves the boson field ψ and an auxiliary dimer field d. The coupling constants g_2 and g_3 are matched to the scattering length and a three-body observable, respectively.

The atom-dimer amplitude is determined by the inhomogeneous integral equation depicted in Fig. 1, where the single lines denote the boson propagator and the double lines denote the full dimer propagator. In a cubic box, the momenta are quantized and the loop integrals in the equation are replaced by discrete sums over quantized momenta $\vec{k} = (2\pi/L) \vec{n}, \vec{n} \in \mathbb{Z}^3$, where L is the side length of the box. The loop sums are regulated via a momentum cutoff Λ just as in the infinite volume case. All observables are independent of Λ . This is achieved by an appropriate dependence of the coupling constant g_3 on Λ [6]. This dependence can be calculated analytically, but one three-body input is required to fix the unknown constant Λ_* (see below). This renormalization procedure is performed in the infinite volume limit. The ultraviolet physics associated with the renormalization of the EFT should not interfere with the infrared physics brought about by putting the system into a finite volume, as long as the corresponding scales are well seperated. We will verify this expectation explicitly below.

FIG. 1: Integral equation for the atom-dimer amplitude. The single lines denote the boson propagator and the double lines denote the full dimer propagator.

The full dimer propagator D denoted by the double lines in Fig. 1 is obtained by dressing the bare dimer propagator which is simply a constant, $4i/g_2$, with bosonic loops. This leads to an infinite sum which can be evaluated analytically yielding

$$D(E, \vec{0}) = \frac{32\pi}{g_2^2} \left[\frac{1}{a} - \sqrt{-E} + \frac{1}{L} \sum_{\substack{\vec{j} \in \mathbb{Z}^3 \\ \vec{j} \neq 0}} \frac{1}{|\vec{j}|} e^{-|\vec{j}|\sqrt{-E}L} \right]^{-1}$$
(3)

for a dimer at rest. The term containing the box length L vanishes in the limit $L \to \infty$ and the expression reduces to the infinite volume result. Using the Feynman rules encoded in Eq. (2) and the full dimer propagator from above, we can translate the Feynman diagrams in Fig. 1 into an equation for the atom-dimer amplitude. It involves an integration over the loop energy and a sum over over the quantized loop momenta. The integration over the loop energy is performed using the residue theorem while the remaining sum over the quantized momenta is rewritten into an integral by virtue of Poisson's resummation formula: $\sum_{\vec{n} \in \mathbb{Z}^3} \delta^3(\vec{z} - \vec{n}) = \sum_{\vec{m} \in \mathbb{Z}^3} \exp(i2\pi\vec{m} \cdot \vec{z}), \text{ which is understood to be used under an integral.}$

The resulting expression is simplified further by exploiting the behavior of the atom-dimer amplitude near a bound state. For energies close to a bound state energy, the amplitude has a simple pole, and the dependence on the ingoing and outgoing momenta seperates. Thus, we obtain a homogeneous integral equation for the bound state amplitude \mathcal{F} , namely

$$\mathcal{F}(\vec{p}) = \frac{1}{\pi^2} \int_{\vec{m} \in \mathbb{Z}^3} d^3 y \sum_{\vec{m} \in \mathbb{Z}^3} e^{iL\vec{m}\cdot\vec{y}} \mathcal{Z}_E(\vec{p}, \vec{y}) \tau_E(y) \mathcal{F}(\vec{y}), \qquad (4)$$

where

$$\mathcal{Z}_{E}(\vec{p}, \vec{y}) = (p^{2} + \vec{p} \cdot \vec{y} + y^{2} - E)^{-1} + \frac{H(\Lambda)}{\Lambda^{2}},$$

$$\tau_{E}(y) = \left(-\frac{1}{a} + \sqrt{\frac{3}{4}y^{2} - E} - \sum_{\vec{j} \in \mathbb{Z}^{3}} \frac{1}{L|\vec{j}|} e^{-L|\vec{j}|\sqrt{\frac{3}{4}y^{2} - E}}\right)^{-1}.$$
(5)

The Λ -dependent three-body interaction in Eq. (5) is given by $H(\Lambda) \equiv -g_3\Lambda^2/(9g_2^2) = \cos[s_0\ln(\Lambda/\Lambda_*) + \arctan s_0]/\cos[s_0\ln(\Lambda/\Lambda_*) - \arctan s_0]$ where $s_0 \approx 1.00624$ is a transcendental number [6].

In the infinite volume case, only S-wave bound states are formed. In a cubic box, however, the extraction of the S-wave part of \mathcal{F} is not straightforward due to the breakdown of the

spherical symmetry to a cubic symmetry. The infinitely many irreducible representations of the spherical symmetry are mapped onto the five irreducible representations of the cubic symmetry. To investigate the mixing of the different partial waves, the part of the amplitude with quantum number ℓ is projected out

$$F_{\ell}(p)c_{\ell 0} = \frac{4}{\pi} \int_{0}^{\Lambda} dy \, y^{2} \left[Z_{E}^{(\ell)}(p,y) \tau_{E}(y) \frac{c_{\ell 0}}{2\ell+1} F_{\ell}(y) + 2\sqrt{\pi} \sum_{\substack{\vec{n} \in \mathbb{Z}^{3} \\ \vec{n} \neq \vec{0}}} \sum_{\ell',m'} \sum_{\ell'',m''} \begin{pmatrix} \ell' & \ell'' & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell' & \ell'' & \ell \\ m' & m'' & 0 \end{pmatrix} \right]$$

$$\times \sqrt{\frac{(2\ell'+1)(2\ell''+1)}{2\ell+1}} i^{\ell''} j_{\ell''}(L|\vec{n}|y) Y_{\ell''m''}(\Omega_{\vec{n}}) Z_E^{(\ell)}(p,y) \tau_E(y) c_{\ell'm'} F_{\ell'}(y) \bigg]$$
(6)

where we have used Wigner 3-j symbols and

$$\frac{Z_E^{(\ell)}(p,y)}{2\ell+1} = \left[\frac{1}{py} Q_\ell \left(\frac{p^2 + y^2 - E}{py} \right) + \frac{H(\Lambda)}{\Lambda^2} \delta_{\ell 0} \right]$$
 (7)

with Q_{ℓ} a Legendre function of the second kind. Moreover, $j_{\ell''}$ is a spherical Bessel function of order ℓ'' . The ℓ'' sum runs over all partial waves while the ℓ' sum runs over partial waves associated with the A_1 representation of the cubic group, namely $\ell' = 0, 4, 6, \ldots$ The size of the contribution of the respective partial wave to the cubic group harmonic of the A_1 representation is given by the coefficients $c_{\ell m}$ (See, e.g., Refs. [29, 30]). The first term in Eq. (6) reproduces the equation for the corresponding partial wave of the infinite volume amplitude, while the second term yields corrections due to the quantization of the momenta and admixtures of other partial waves.

For our study of the trimer states in the cubic box, this equation is now specialized to the $\ell = 0$ case:

$$F_0(p) = \frac{4}{\pi} \int_0^{\Lambda} dy \, y^2 Z_E^{(0)}(p, y) \tau_E(y) \left(1 + \sum_{\vec{n} \in \mathbb{Z}^3 \atop \vec{n} \neq \vec{0}} \frac{\sin(L|\vec{n}|y)}{L|\vec{n}|y} \right) F_0(y) + \dots, \tag{8}$$

where the dots indicate admixtures from higher partial waves. Since the leading term in the expansion of the Bessel functions in Eq. (6) is $1/(L|\vec{n}|y)$ these contributions are suppressed by at least a/L. They will be small for volumes not too small compared to the size of the bound state. The lowest partial wave that is mixed with the S-wave is the $\ell=4$ wave. Moreover, contributions from higher partial waves will be suppressed kinematically for shallow states with small binding momentum. This is ensured by the spherical harmonic in the second term of Eq. (6). Only for small lattices, i. e. when a/L is large, this behavior is counteracted by terms stemming from the spherical Bessel function $j_{\ell}(L|\vec{n}|y)$ and higher partial waves may contribute significantly. We will therefore only consider the terms explicitly given in Eq. (8) and leave the calculation of corrections due to higher partial waves for future work. For the numerical solution of Eq. (8), a set of basis functions is chosen to turn the integral equation into a homogeneous matrix equation. The basis functions chosen are shifted Legendre polynomials defined on the intervall $[0,\Lambda]$ with a logarithmic dependence in the argument. This behavior is tailored to the known log-periodic behavior of the infinite volume bound state amplitude [6]. The set of basis functions is orthonormal with respect to a suitable chosen scalar product. The energy E is now varied such that the resulting matrix

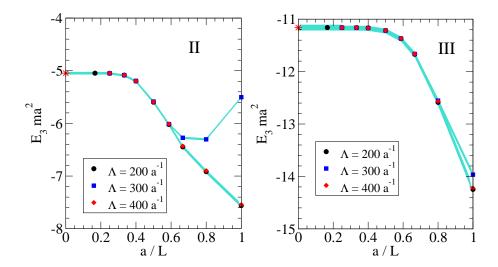


FIG. 2: Variation of the trimer energy E_3 with the length L of the cubic volume for the states II (left) and III (right). Plotted are three datasets for different values of the cutoff parameter Λ , together with the $1/(\Lambda a)$ bands. The point a/L = 0 corresponds to the infinite volume limit.

has the eigenvalue one. In order to reduce the numerical effort, a Taylor expansion of the integral kernel

$$Z_E^{(0)}(p,y)\tau_E(y) = Z_{E_3^{\infty}}^{(0)}(p,y)\tau_{E_3^{\infty}}(y) + \frac{\mathrm{d}}{\mathrm{d}E} Z_E^{(0)}(p,y)\tau_E(y)\Big|_{E=E_3^{\infty}} (E - E_3^{\infty}) + \mathcal{O}\left((E - E_3^{\infty})^2\right)$$
(9)

around the infinite volume energy E_3^{∞} is performed. In the following, we consider only the linear term in this expansion. We expect this approximation to be valid for small energy shifts; its validity will be discussed in detail below. More details on the numerical method will be presented in a forthcoming publication.

For this first study of the trimer energies in a cubic box, we take a > 0 and choose four states that have different energies in the infinite volume including shallow as well as deep states:

Ia:
$$E_3^{\infty} = -1.18907/a^2$$
, $\Lambda_* a = 5.66$

Ib:
$$E_3^{\infty} = -27.4427/a^2$$
, $\Lambda_* a = 5.66$,

II:
$$E_3^{\infty} = -5.04626/a^2$$
, $\Lambda_* a = 1.66$

III:
$$E_3^{\infty} = -11.1322/a^2$$
, $\Lambda_* a = 3.66$,

where E_3^{∞} is the trimer energy in the infinite volume. Note that the states Ia and Ib appear in the same physical system characterized by $\Lambda_* a = 5.66$.

For each of these states, the energy in finite volume has been calculated for various L. Our results are shown in Figs. 2 and 3. In order to check the consistency of our results, the calculation was carried out for several cutoff momenta Λ and proper renormalization was verified explicitly. For each cutoff the three-body interaction $H(\Lambda)$ was adjusted to give the correct energy in infinite volume. The calculated values in Figs. 2 and 3 agree with each other very well within the depicted error bands of the size $1/(\Lambda a)$ as long as the finite volume energy shift is not larger than 15–20% of the infinite volume energy. These error bands give

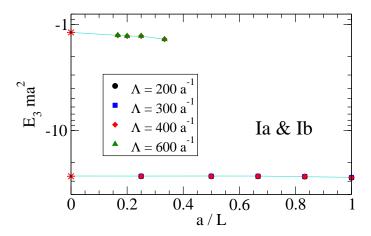


FIG. 3: Variation of the trimer energy E_3 with L for the states Ia (upper curves) and Ib (lower curves). Plotted are two (three) datasets for different values of Λ , together with the $1/(\Lambda a)$ bands.

an estimate of the finite cutoff corrections and renormalized quantities have to agree within these errors. They do not correspond to the error from higher order corrections in the EFT.

When the finite volume shifts become larger than 15–20% of the infinite volume energy, the calculated results for different cutoffs in Fig. 2 start to disagree and proper renormalization cannot be achieved anymore. For the shallower state II this occurs for $a/L \approx 0.6$ while the deeper state III can be treated in the linear approximation up to $a/L \approx 0.85$. This behavior of the energy shift for the shallow states indicates the breakdown of the Taylor expansion of the integral kernel. As expected, the linear approximation in Eq. (9) is not applicable anymore if the finite volume shift becomes to large. Calculations that do not rely on this expansion require a higher numerical effort. Such calculations are currently performed and the results will be presented in a forthcoming publication.

In Fig. 3, we show our results for the two states Ia and Ib in the same system characterized by $\Lambda_* a = 5.66$ for box sizes where the linear approximation in the kernel is justified. For the shallowest state Ia reliable results can not be obtained for box sizes L < 3a while for the deepest state Ib no appreciable finite volume shift can be detected for L > a. Generally, the L dependence of the energy shows a similar behavior for all investigated states. For large box sizes, the finite volume energy agrees with the infinite volume value. If the box size is decreased, the binding increases. The finite volume corrections are most important for the shallowest states which are largest in size and feel the finite volume first. For example, the ratio of the energies of the states Ia and Ib decreases from 23.08 in the infinite volume limit to 19.5 for L = 3a. Note that this ratio differs from the discrete scaling factor $\exp(2\pi/s_0) \approx 515$ even in the infinite volume limit. This behavior is expected for shallow states close to the bound state threshold [3]. The ratio $\exp(2\pi/s_0)$ will be approached if deeper states are considered.

In this letter, we have studied the Efimov spectrum of three bosons in a cubic box with periodic boundary conditions. The knowledge of these modifications is important in order to understand results from future 3-body lattice calculations. Using the framework of EFT, we derived a general equation for the trimer energies in the box. We solved this equation for box sizes as small as L=a in a linear approximation of the kernel for small finite volume shifts and studied the modifications of the spectrum as the system is squeezed into the box. Moreover, we investigated the breakdown of the linear approximation. We find that the

expanded kernel seems to be applicable as long as the finite volume shift in the energy is not larger than 15–20% of the infinite volume energy. Numerically more expensive calculations using the unexpanded equation are under way. As a next step, the role of the higher partial waves contributing to the bound state amplitude has to be investigated in detail. This might allow to push the calculations to even smaller volumes and the regime L/a < 1 similar to the two-body system [28]. Finally, our method should be extended to the three-nucleon system in order to be able to test the conjecture of Ref. [16] in the future. This requires also the inclusion of higher order corrections in the EFT and finite temperature effects as lattice calculations will inevitably be performed at a small, but non-zero, temperature.

This research was supported by the DFG through SFB/TR 16 "Subnuclear structure of matter" and the BMBF under contract No. 06BN411.

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